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"Spall-4:" An Energy-Based Model for Spall (U)

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An energy-dependent bond-breaking model for material failure is described. The logic of the scheme has its roots in that of the Cochran-Banner spall model [Cochran and Banner, 1977], but significant differences have been introduced. Material zones undergoing tensile stress incur damage according to an exponential expression related to the familiar Maxwell-Boltzmann distribution. A scheme for converting the damage calculated in specified contiguous zones of the mesh into a "strength factor" for each subject zone is included as a means to account for statistical variability in the location and extent of the failure region. A dynamical healing algorithm is also described. To date the method has been tried only in 1-D slab symmetry, but it is intended for general use in mesh-zoned hydro codes of any dimensionality. (U)

Introduction

The spall-4 material failure model grows out of the realization that, if sufficient tensile work is done on a cohesive material, it will rupture. Furthermore, if the material approaches failure along an isentrope (as we assume), then its path to failure might be reproducible to within some appropriate degree of accuracy. If so, then failure ought to be susceptible to description in terms of the thermodynamic variables that we utilize in our codes.

The spall-4 model in its current form constitutes a first attempt at pursuing this notion. Nominal functional forms are adduced to represent (1) the amount of damage that might accumulate in a zone of condensed material as a result of work done on it by tensile stresses, and (2) the amount of healing that might take place under various combinations of heating and compression. Variations in experimental results obtained using nominally similar materials indicates the presence of important randomizing influences, which in turn suggests that some sort of statistical weighting scheme might be called for when calculating the effects of the zonal damage. We should expect this to be especially important in highly resolved 1-D calculations. A method that involves averaging the damage over a stencil of contiguous zones to get a resultant strength factor for the central member of the stencil is therefore included as part of the overall treatment.

The Spall-4 Model

Dynamics

A conceptual jumping-off point for envisioning the onset of failure in this model is to picture the material as a collection of atoms connected pairwise by electronic potential energy bonds that are anharmonic functions of the atomic separation. These bonds are characterized by a definite dissociation energy. A bond elongated beyond some criterion limit will have enough energy to be considered dissociated, and a bond with that amount of energy is therefore considered broken regardless of elongation. If a sufficient number of bonds in a mesh zone of the material meet or exceed the criterion energy of dissociation, the material in that zone will not be able to support a tension and the zone will be considered failed.

To get a handle on the fraction of the bonds that have to break for failure to be complete, consider a simple cubic lattice oriented along the (x,y,z) coordinate directions. If a uniform tension is applied normal to the (x,y) plane, then only bonds in the z-direction have to break for failure to occur. In the simple cubic model posed here, that means the bond-breaking fraction at failure will be 1/3. Now, we don't expect the structure of real materials to be simple, uniform, or conveniently oriented, but 1/3 nevertheless seems like a reasonable value for the initial estimate of a failure fraction. Then β, the first parameter of the model, defined to be the inverse of the bond failure fraction, will have default value 3.

The next need is to estimate the fraction of the bonds that have energy greater than the dissociation energy. We write this assuming a sort of quasi-Maxwell-Boltzmann energy distribution,

$$f_b = \exp [E_{diss} / (E - E_x)], \qquad [1]$$

where E_{diss} is the energy per gram needed for dissociation and E is the internal energy of the material

E_{diss} and E_x are not definite at this point. As of this writing, E_x is the internal energy remembered from the moment the material passed into tension and E_{diss} is a user-input constant modified by a melt function. For single-stage spall, with no intervening recompression followed by renewed tension, this may do as an empiricism, but it isn't really satisfactory. This is one aspect of the model that is being worked actively at this time. Further comment is reserved for the Discussion and Conclusions section ahead.

In any case, E_x is a quantity that depends on the state of the material at some point in the calculation and so is not input by the user. Damage for the k^{th} zone is given as

$$\text{damage} (k) = \beta * f_b = \beta * \exp [E_{diss} / (E - E_x)]. \qquad [2]$$

This quantity ratchets. That is, if the energy accumulated in tension exceeds a user-specified value E_{infl}, or if the damage at some point exceeds a noise threshold *damth* (cur-

rently 5%, not a user input), then the damage is not allowed to decrease thereafter except via the model's healing algorithm. E_{infl} is the third input parameter of the model.

Healing can occur when the zone pressure is positive. Three categories of healing are admitted: melt, crushup, and thermal.

Melt healing is the simplest: if a zone is melted and P>0, then the zone is considered healed; that is, if the zone subsequently resolidifies and passes back into tension, the material in it will be treated as undamaged.

Crushup healing occurs when the material is solid and the pressure exceeds the material parameter *pcrush*. It is a simple rate process:

$$d(\text{damage}) / dt = -\gamma * \text{damage}. \qquad [3]$$

The crushup rate parameter γ is the fourth user input parameter.

Thermal healing occurs when the pressure is positive but less than the crush pressure. It is based on the notion that some dislocation features will be mobile, and that of these some fraction will interact with material features so as to resolve themselves. The thermal healing expression is

$$d(\text{damage}) / dt = -\alpha * g(E_{th}) * \text{damage}. \qquad [4]$$

The thermal rate parameter α is the fifth user input parameter. E_{th} is the thermal energy per unit mass in the zone and the function g is a more typical Maxwell-Boltzmann expression,

$$g(E_{th}) = \exp[-E_{heal} / E_{th}]. \qquad [5]$$

E_{heal} is the sixth user input parameter.

With the damage in zone k calculated for a given hydro cycle, a strength multiplier is calculated. At first blush we might write

$$f_{sm}(k) = 1 - \text{damage}(k)^{2/3}, \qquad [6]$$

where the exponent 2/3 is chosen consistent with failure via the growth of spherical voids. f_{sm} starts out unity. As the damage approaches 1, f_{sm} goes to zero. The yield strength and the shear modulus are multiplied by this factor. If the zone is in tension, the pressure and bulk modulus are likewise reduced. Thus f_{sm} is the means by which the model represents the effect of spall on the system hydro. As it stands, however, the damage proves rather highly localized; too much so for Eq. [6] to be satisfactory. It is necessary to take some account of nature's inexactitude.

The strength multiplier: Damage weighting

The interior surface of a spall scab or blister is not very smooth, certainly not on the few-micron scale. To get a good representation of the model dynamics, however, we often have to use a very highly resolved mesh. The 1-D calculations carried out in aid of the present work, for example, consistently resorted to 5-micron zoning. However, in-

cipient-spall experiments show damage arising more or less randomly over distances some five times as great as that, while full-up spall in gasgun experiments results in damage in the sample over a region comparable to the size of the flyer. Spall-4 calculations that do not include some means to fuzz over the damage calculated in the individual zones have shown excessively localized results. In this section I present a method for taking into account the statistical nature of real materials' failure dynamics. The method has also proven effective in smoothing the hydro as damage accumulates.

The Cochran-Banner model started out facing the same issue of undue localization of calculated spall effects. Accordingly, the initial formula for converting damage to the strength multiplier f_{sm} was subsequently modified to take damage in neighboring zones into account:

$$fs = damage(k-1) + damage(k) + damage(k+1), \quad [7']$$

$$fd = \min(fs, 1), \quad [8]$$

$$f_{sm}(k) = 1 - fd^{2/3}. \quad [9']$$

There are drawbacks to this approach, however, as can easily be seen. For example, a perfectly unspalled zone can have moderate spall on either side of it and find itself represented as being practically destroyed. Therefore I have modified the scheme by introducing weights for the various damage contributions and so arrive at a different expression for the intermediate quantity fs:

$$fs = wm*damage(k-1) + wz*damage(k) + wp*damage(k+1). \quad [7]$$

The weights add up to one. They are calculated first by looking at dr(k), the size of the k^{th} zone, in comparison with the size of a maximum elongation dam0, which is a material property carried in our databases. The basic algorithm is easily expressed:

```
If  ( dr(k) > dam0 )  then
    wz  =  1  -  dam0 / ( 3*dr(k) )
Else
    wz  =  ( 1  +  dr(k) / dam0 ) / 3
Endif
wz  =  max ( wz, damage(k) )
If  ( wz > 0.99 )  then
    wm  =  0;  wz  =  1;  wp  =  0
Else
    wm  =  wp  =  0.5 * ( 1 – wz )
Endif
```

Special cases are easily derived to treat boundary zones. Note that, for nonzero dr, wz is always bound between 1/3 and 1. In the limit of zero thickness, damage is equally weighted over the three contiguous zones.

It is easy to imagine improving on this weighting scheme by adding mechanisms for nucleating and diffusing dislocation structures. It may still be necessary to take explicit account of the statistical uncertainties that abound in real materials, but even so, this is a fruitful area for future development of the model.

A further modification to the strength multiplier has shown interesting effects. In place of Eq. [9'] we write

$$f_{sm}(k) = 1 - fd^{damexp}, \qquad [9]$$

where the exponent defaults to 2/3 as before. Smaller values of *damexp* cause a faster initial reduction in f_{sm}, but this in turn keeps the energy in the zone from building as rapidly as it would if the stress in the zone were not being reduced so much. The upshot is, that the zone actually stretches out further before failing than would be the case with a larger value of the exponent. This mimics something of what we would expect from a more ductile material, and together with modifications to the β-parameter, it offers a way to explore sensitivity of the model to ductility variations.

Calculations

The model has been compared with some of the copper-on-copper gasgun shots carried out by Mukul Kumar as part of the lab's material failure modeling effort. Here we focus on one of these, shot 857, in which a 1.5mm copper flyer impacts at velocity 1277 m/sec = 0.1277 cm/microsec on a 4-mm copper sample. The data to be compared are the simulated and experimentally observed velocity traces from the front surface of the sample.

Fig. 1 shows the simulated velocity trace obtained using the new model. A series of peaks are observed, decreasing in height as time increases until a climax shape is achieved at about the fifth excursion. The calculated release behavior from the first maximum shows a distinct step. This reflection of the elastic precursor suggests a shortcoming of the Steinberg-Guinan constitutive model (Steinberg *et al.*, 1980) when used in this context. We do not see a corresponding step in the experimental record.

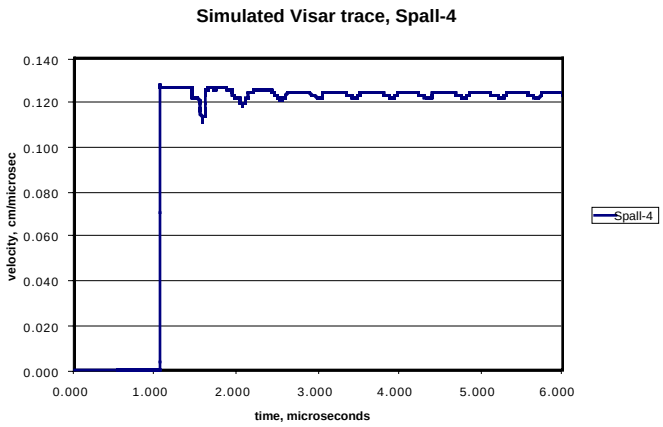
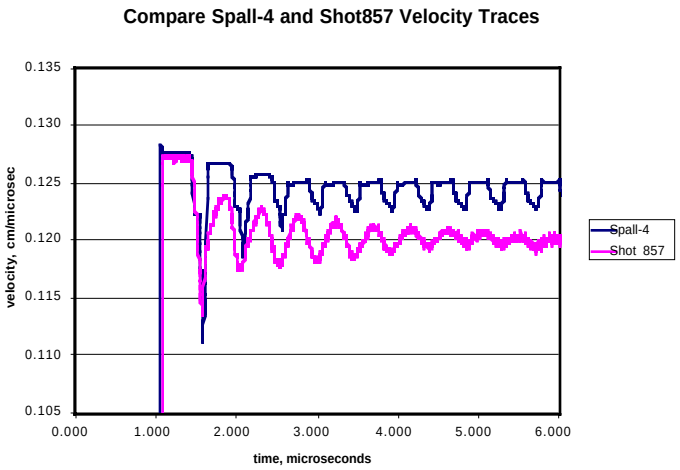


Fig. 1. Front-surface velocity of copper sample vs. time from 1-D simulation of copper shot 857 using spall-4 failure model. Time is in μsec and velocity is in cm/μsec.

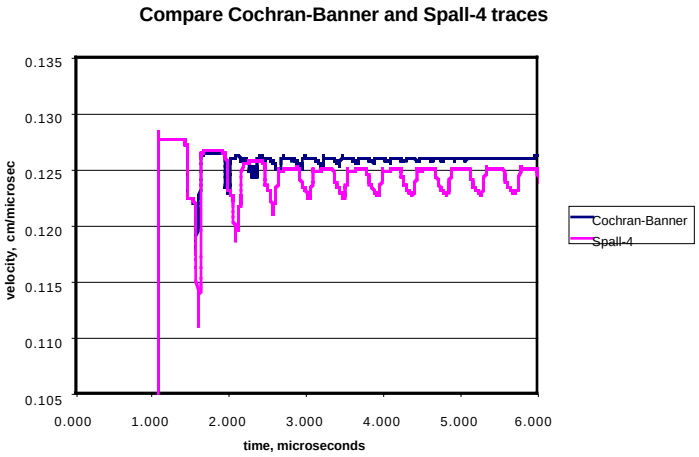
In Fig. 2 we superimpose the experimental record on the spall-4 calculation to make a more direct comparison. We see that the experimental peaks (lower curve, pink) look much different than their computed counterparts, although their periodicity is well reproduced by the model. The calculation appears to leave too much energy in the material, so that it rebounds much more sharply and to a significantly greater degree than is evidenced in the experimental record. Also, the experimental peaks continue to decline all across the record, well after the calculation has settled into a final profile. Tentatively, as indicated above, I attribute at least some of the difference to shortcomings in the copper EOS and in the constitutive model that I used. One of my near-term goals is to repeat the work using other representations of the material properties.

Fig. 2. Comparison of spall-4 and experimental velocity records for shot 857. The velocity range of the plot is from 0.105 to 0.135 cm/μsec.



Finally, in Fig. 3 we compare results from the Cochran-Banner and spall-4 models. The most obvious difference is the rapidity with which the velocity trace obtained using the older model smooths out with time. The periodicity of the peak structure is significantly shorter, too, indicating that the damage region reaches much closer to the front surface than with the spall-4 treatment. The final velocity lies distinctly above that of the spall-4 trace, although the difference represents only another 2 or 3% error relative to the experiment.

Fig. 3. Comparison between Cochran-Banner and Spall-4 model results. Velocity range is as in Fig. 2.



Discussion and Conclusions

Our problem with determining values for the parameters E_{diss} and E_x that appear in the energy distribution function of Eq. [1] might go away if we could project good effective isentropes for the EOS when the material goes into tension. E_x might then be the minimum of the material's cold curve, for example, and E_{diss} the difference between the maximum of the dissociation isentrope and E_x. If these or some similar assignments

work, then E_{diss} and E_x would neither one be input by the user; rather, both would be part of the hydro calculation.

The model as currently run includes other user inputs, most notably the parameters a_{diss} and f_{diss} which are used in a function that modifies E_{diss} and E_{infl} as the material approaches melt. These and related forms are not central to the model and so are not discussed here in any detail, but the fact that real materials do melt, for example, means that at some point, if the model shows sufficient utility, these kinds of considerations will have to be taken seriously.

Work to date has been carried out in 1-D only, but the model is intended for general use. Two considerations naturally arise when we contemplate its incorporation in any of our higher-dimensioned ALE codes: Is the model in any way directional; i.e., does it depend on any vector or tensor quantities? And what are its history variables and how might we expect them to behave under advection? Not yet having attempted the 2-D or 3-D implementations, I am not able to say with certainty that the model will work there, but my expectation that it will work is not unreasonable. First, it does not depend on directional quantities for its dynamics. It uses familiar thermodynamic quantities such as pressure, energy, temperature, and phase (when melt is an issue) to evolve the damage state. With regard to advection, it should be no harder to treat the damage fraction than it is to treat, say, the burn fraction in detonating HE. Everything else in the model is derived during the current hydro step and so does not have to be advected at all.

Parallel work here at LLNL and elsewhere has been concentrating on understanding porosity and how it leads to material failure. I hope that my approach represents a useful connection between porosity-based analyses and failure modeling in the codes. As we get a better understanding of the energetics involved in porosity and dislocation dynamics, we might hope to discover correlations that show how to improve the model's ability to represent the effects of material failure.

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Disclaimer

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